

# 4-(4-Chlorophenyl)-4-hydroxypiperidinium benzoate

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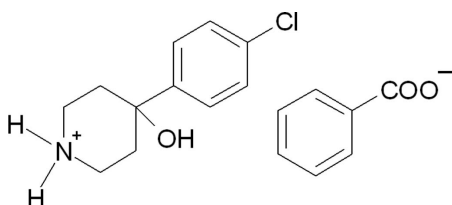
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Key indicators: single-crystal X-ray study;  $T = 173$  K; mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å;  $R$  factor = 0.046;  $wR$  factor = 0.125; data-to-parameter ratio = 19.3.

In the title salt,  $\text{C}_{11}\text{H}_{15}\text{ClNO}^+\cdot\text{C}_7\text{H}_5\text{O}_2^-$ , the dihedral angle between the mean planes of the chlorophenyl ring of the cation and the benzene ring of the anion is  $74.4(1)^\circ$ . In the cation, the six-membered piperazine ring adopts a chair conformation. The crystal packing is stabilized by intermolecular  $\text{N}-\text{H}\cdots\text{O}$  and  $\text{O}-\text{H}\cdots\text{O}$  hydrogen bonds, and weak intermolecular  $\text{C}-\text{H}\cdots\text{O}$ ,  $\text{C}-\text{H}\cdots\text{Cl}$  and  $\text{C}-\text{H}\cdots\pi$  interactions.

## Related literature

For the synthesis and biological activity of uncondensed cyclic derivatives of piperidine, see: Vartanyan (1984). For puckering parameters, see: Cremer & Pople (1975). For related structures, see: Jasinski *et al.* (2009). For ring-motif patterns, see: Bernstein *et al.* (1994).



## Experimental

### Crystal data

$\text{C}_{11}\text{H}_{15}\text{ClNO}^+\cdot\text{C}_7\text{H}_5\text{O}_2^-$   
 $M_r = 333.80$   
Triclinic,  $P\bar{1}$   
 $a = 9.6235(12)$  Å  
 $b = 10.0971(16)$  Å  
 $c = 10.2251(14)$  Å  
 $\alpha = 99.608(12)^\circ$   
 $\beta = 108.748(13)^\circ$   
 $\gamma = 113.357(14)^\circ$   
 $V = 812.7(2)$  Å<sup>3</sup>

$Z = 2$   
Mo  $K\alpha$  radiation  
 $\mu = 0.25\text{ mm}^{-1}$

$T = 173$  K  
 $0.34 \times 0.30 \times 0.13$  mm

### Data collection

Oxford Diffraction Xcalibur Eos  
Gemini diffractometer  
Absorption correction: multi-scan  
(*CrysAlis RED*; Oxford  
Diffraction, 2010)  
 $T_{\min} = 0.920$ ,  $T_{\max} = 0.968$

7857 measured reflections  
4184 independent reflections  
3222 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.018$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.046$   
 $wR(F^2) = 0.125$   
 $S = 1.05$   
4184 reflections  
217 parameters  
4 restraints

H atoms treated by a mixture of  
independent and constrained  
refinement  
 $\Delta\rho_{\max} = 0.29\text{ e \AA}^{-3}$   
 $\Delta\rho_{\min} = -0.34\text{ e \AA}^{-3}$

Table 1

Hydrogen-bond geometry (Å, °).

Cg3 is the centroid of the C13–C18 ring.

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N1}-\text{H1N}^+\cdots\text{O3}^{\text{i}}$	0.87 (1)	1.84 (1)	2.6964 (17)	166 (2)
$\text{O1}-\text{H1O}\cdots\text{O3}$	0.82 (2)	2.05 (2)	2.7780 (16)	147 (2)
$\text{N1}-\text{H1N}^+\cdots\text{O2}^{\text{ii}}$	0.86 (1)	1.92 (1)	2.7609 (18)	166 (2)
$\text{C16}-\text{H16A}\cdots\text{C11}^{\text{iii}}$	0.95	2.78	3.5268 (17)	136
$\text{C9}-\text{H9B}\cdots\text{O1}^{\text{i}}$	0.99	2.46	3.3008 (19)	143
$\text{C1}-\text{H1A}\cdots\text{Cg3}^{\text{iv}}$	0.95	2.70	3.554 (2)	150

Symmetry codes: (i)  $-x+1, -y+1, -z+2$ ; (ii)  $x, y-1, z$ ; (iii)  $-x, -y+1, -z$ ; (iv)  $-x, -y+1, -z+1$ .

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2010); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2415).

## References

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## supporting information

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**4-(4-Chlorophenyl)-4-hydroxypiperidinium benzoate**

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**S1. Comment**

4-(4-Chlorophenyl)-4-hydroxypiperidine is used as an intermediate for the synthesis of pharmaceuticals such as haloperidol (a neuroleptic drug used to treat patients with psychotic illnesses, extreme agitation, or Tourette's syndrome) and loperamide (a synthetic piperidine derivative, effective against diarrhea resulting from gastroenteritis or inflammatory bowel disease). A review on the synthesis and biological activities of uncondensed cyclic derivatives of piperidine is reported (Vartanyan, 1984). The crystal structure of a related compound, 4-[(E)-(2,4-difluorophenyl) (hydroxyimino)methyl]piperidinium picrate (Jasinski *et al.*, 2009) has been reported. In this paper we report the crystal structure of  $C_{11}H_{15}ONCl^+ \cdot C_7H_5O_2^-$ .

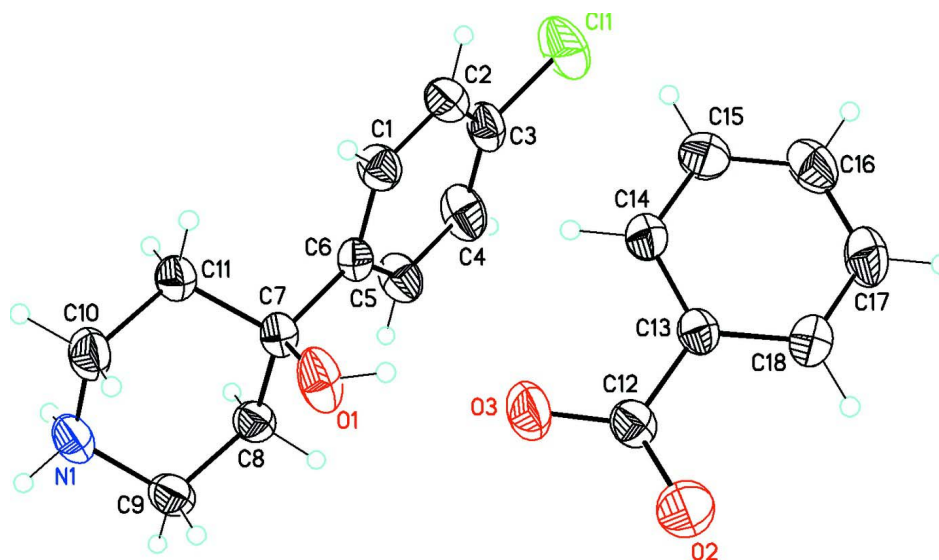
In the title salt (Fig. 1), the 6-membered piperazine ring in the cation adopts a chair conformation with puckering parameters (Cremer & Pople, 1975)  $Q$ ,  $\theta$  and  $\varphi$ , 0.568 (2) Å, 0.00 (19)° and 278 (9)°, respectively. The dihedral angle between the mean planes of the chlorophenyl ring of the cation and the benzene ring of the anion is 74.4 (1)°. The crystal structure is stabilized by N1—H1NA...O3 and N1—H1NB...O2, hydrogen bonds forming  $R_4^4(12)$  ring-motif pattern (Bernstein *et al.*, 1994) and N1—H1NA...O3, O1—H10...O3 hydrogen bonds resulting in  $R_2^4(16)$  ring-motif, generating one dimensional chains along the  $c$  axis (Fig. 2). The structure is further consolidated by weak C9—H9B...O1, C16—H16A...Cl1 and C1—H1A...Cg3  $\pi$ -ring intermolecular interactions.

**S2. Experimental**

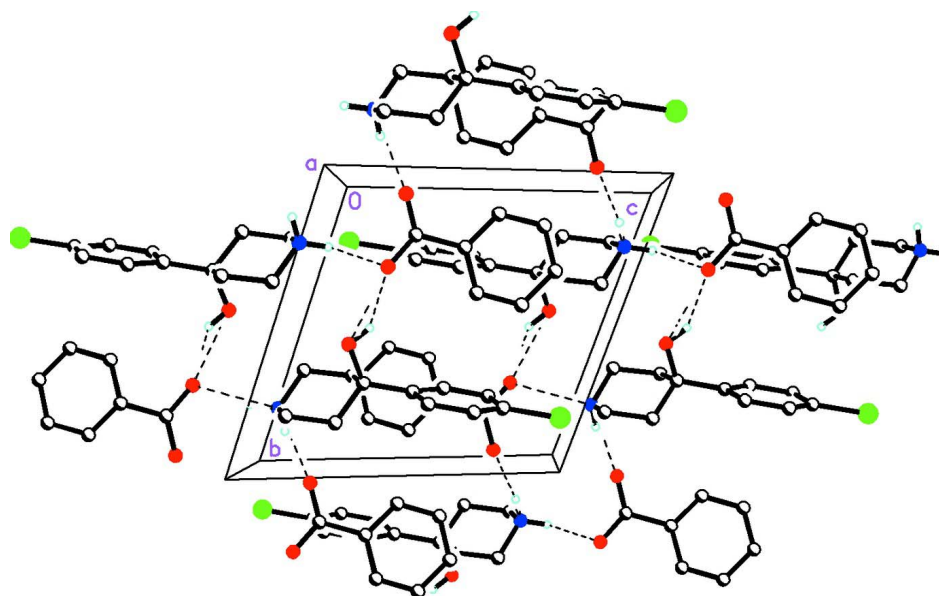
Solutions of 4-(4-chlorophenyl)-piperidin-4-ol (2.12 g, 0.01 mol) in methanol (10 ml) and benzoic acid (1.226 g, 0.01 mol) in methanol (10 ml) were mixed and stirred in a beaker at 333 K for 30 minutes. The mixture was kept aside for three days at room temperature. The salt thus obtained was filtered and dried in a vacuum desiccator over phosphorous pentoxide. The compound was recrystallized from N,N-dimethylformamide by slow evaporation (m.p: 498 - 501 K).

**S3. Refinement**

Hydrogen atoms on O1 and N1 were found from a Fourier difference map and were refined using DFIX 0.84(0.02) and 0.86(0.01) values for O—H and N—H distances, respectively, and  $U_{iso}(H) = 1.2$  times  $U_{eq}(O/N)$ . The rest of the H atoms were positioned geometrically, and allowed to ride on their parent atoms, with C—H distances 0.95 Å (CH) or 0.99 Å (CH<sub>2</sub>) and  $U_{iso}(H) = 1.18$ - $1.21$  times  $U_{eq}(C)$ .

**Figure 1**

Molecular structure of the title compound showing the atom labeling scheme and 50% probability displacement ellipsoids.

**Figure 2**

Packing diagram for the title compound viewed down the *a* axis. Dashed lines indicate N—H...O and O—H...O hydrogen bonds generating one dimensional chains along the *c* axis.

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##### Crystal data

$C_{11}H_{15}ClNO^+ \cdot C_7H_5O_2^-$

$M_r = 333.80$

Triclinic,  $P\bar{1}$

Hall symbol: -P 1

$a = 9.6235$  (12) Å

$b = 10.0971$  (16) Å

$c = 10.2251$  (14) Å

$\alpha = 99.608$  (12)°

$\beta = 108.748$  (13)°

$\gamma = 113.357$  (14)°

$V = 812.7 (2) \text{ \AA}^3$   
 $Z = 2$   
 $F(000) = 352$   
 $D_x = 1.364 \text{ Mg m}^{-3}$   
 Mo  $K\alpha$  radiation,  $\lambda = 0.71073 \text{ \AA}$   
 Cell parameters from 3721 reflections

$\theta = 3.7\text{--}32.3^\circ$   
 $\mu = 0.25 \text{ mm}^{-1}$   
 $T = 173 \text{ K}$   
 Block, colorless  
 $0.34 \times 0.30 \times 0.13 \text{ mm}$

#### Data collection

Oxford Diffraction Xcalibur Eos Gemini  
 diffractometer  
 Radiation source: Enhance (Mo) X-ray Source  
 Graphite monochromator  
 Detector resolution:  $16.1500 \text{ pixels mm}^{-1}$   
 $\omega$  scans  
 Absorption correction: multi-scan  
 (*CrysAlis RED*; Oxford Diffraction, 2010)  
 $T_{\min} = 0.920$ ,  $T_{\max} = 0.968$

7857 measured reflections  
 4184 independent reflections  
 3222 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.018$   
 $\theta_{\max} = 28.7^\circ$ ,  $\theta_{\min} = 3.7^\circ$   
 $h = -12 \rightarrow 12$   
 $k = -13 \rightarrow 13$   
 $l = -13 \rightarrow 13$

#### Refinement

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.046$   
 $wR(F^2) = 0.125$   
 $S = 1.05$   
 4184 reflections  
 217 parameters  
 4 restraints  
 Primary atom site location: structure-invariant  
 direct methods

Secondary atom site location: difference Fourier  
 map  
 Hydrogen site location: inferred from  
 neighbouring sites  
 H atoms treated by a mixture of independent  
 and constrained refinement  
 $w = 1/[\sigma^2(F_o^2) + (0.0558P)^2 + 0.1776P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.29 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\min} = -0.34 \text{ e \AA}^{-3}$

#### Special details

**Geometry.** All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

**Refinement.** Refinement of  $F^2$  against ALL reflections. The weighted  $R$ -factor  $wR$  and goodness of fit  $S$  are based on  $F^2$ , conventional  $R$ -factors  $R$  are based on  $F$ , with  $F$  set to zero for negative  $F^2$ . The threshold expression of  $F^2 > \sigma(F^2)$  is used only for calculating  $R$ -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement.  $R$ -factors based on  $F^2$  are statistically about twice as large as those based on  $F$ , and  $R$ -factors based on ALL data will be even larger.

#### Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
Cl1	0.01350 (8)	0.19249 (7)	0.06335 (5)	0.06605 (19)
O1	0.37436 (18)	0.44147 (14)	0.79300 (12)	0.0470 (3)
H1O	0.360 (3)	0.498 (2)	0.746 (2)	0.056*
O2	0.46446 (18)	0.94763 (13)	0.77613 (13)	0.0553 (4)
O3	0.36182 (17)	0.70222 (13)	0.75160 (12)	0.0504 (3)
N1	0.51659 (18)	0.21683 (15)	0.95370 (13)	0.0372 (3)
H1NB	0.514 (2)	0.1342 (16)	0.9106 (18)	0.045*
H1NA	0.561 (2)	0.231 (2)	1.0473 (12)	0.045*
C1	0.1141 (2)	0.24120 (18)	0.48209 (16)	0.0351 (3)

H1A	0.0551	0.2344	0.5416	0.042*
C2	0.0314 (2)	0.21412 (19)	0.33410 (17)	0.0393 (4)
H2A	-0.0832	0.1888	0.2920	0.047*
C3	0.1181 (2)	0.22451 (18)	0.24891 (16)	0.0387 (4)
C4	0.2839 (2)	0.2611 (2)	0.30731 (18)	0.0474 (4)
H4A	0.3419	0.2678	0.2470	0.057*
C5	0.3653 (2)	0.2881 (2)	0.45636 (17)	0.0404 (4)
H5A	0.4802	0.3140	0.4978	0.048*
C6	0.28210 (18)	0.27817 (15)	0.54568 (14)	0.0278 (3)
C7	0.36689 (18)	0.30769 (15)	0.70961 (14)	0.0282 (3)
C8	0.54504 (19)	0.32943 (17)	0.76015 (15)	0.0331 (3)
H8A	0.5421	0.2395	0.7006	0.040*
H8B	0.6156	0.4212	0.7432	0.040*
C9	0.6232 (2)	0.34823 (18)	0.92121 (16)	0.0373 (3)
H9A	0.7351	0.3556	0.9474	0.045*
H9B	0.6383	0.4445	0.9818	0.045*
C10	0.3447 (2)	0.19647 (19)	0.91069 (16)	0.0388 (4)
H10A	0.3496	0.2880	0.9697	0.047*
H10B	0.2763	0.1064	0.9310	0.047*
C11	0.26339 (19)	0.17363 (18)	0.74911 (16)	0.0346 (3)
H11A	0.1503	0.1632	0.7235	0.042*
H11B	0.2503	0.0774	0.6904	0.042*
C12	0.37590 (19)	0.80987 (17)	0.70139 (15)	0.0324 (3)
C13	0.27602 (18)	0.76646 (16)	0.53903 (15)	0.0283 (3)
C14	0.1622 (2)	0.61404 (17)	0.45411 (16)	0.0363 (3)
H14A	0.1524	0.5367	0.4977	0.044*
C15	0.0633 (2)	0.5739 (2)	0.30681 (18)	0.0447 (4)
H15A	-0.0151	0.4695	0.2498	0.054*
C16	0.0782 (2)	0.6857 (2)	0.24240 (18)	0.0463 (4)
H16A	0.0093	0.6580	0.1413	0.056*
C17	0.1924 (2)	0.8366 (2)	0.32407 (19)	0.0452 (4)
H17A	0.2042	0.9130	0.2790	0.054*
C18	0.2902 (2)	0.87754 (17)	0.47237 (17)	0.0360 (3)
H18A	0.3677	0.9823	0.5289	0.043*

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Cl1	0.0874 (4)	0.0854 (4)	0.0294 (2)	0.0485 (3)	0.0179 (2)	0.0257 (2)
O1	0.0826 (9)	0.0447 (7)	0.0316 (6)	0.0468 (7)	0.0235 (6)	0.0149 (5)
O2	0.0710 (9)	0.0364 (6)	0.0391 (6)	0.0248 (6)	0.0082 (6)	0.0014 (5)
O3	0.0727 (9)	0.0397 (6)	0.0299 (5)	0.0272 (6)	0.0101 (6)	0.0147 (5)
N1	0.0512 (8)	0.0349 (7)	0.0253 (6)	0.0256 (6)	0.0101 (6)	0.0098 (5)
C1	0.0360 (8)	0.0427 (8)	0.0311 (7)	0.0198 (7)	0.0169 (6)	0.0158 (6)
C2	0.0362 (8)	0.0442 (9)	0.0344 (7)	0.0189 (7)	0.0109 (7)	0.0159 (7)
C3	0.0526 (10)	0.0401 (8)	0.0270 (7)	0.0256 (8)	0.0151 (7)	0.0155 (6)
C4	0.0594 (11)	0.0691 (12)	0.0375 (8)	0.0397 (10)	0.0314 (8)	0.0291 (8)
C5	0.0406 (9)	0.0589 (10)	0.0371 (8)	0.0300 (8)	0.0225 (7)	0.0243 (7)

C6	0.0346 (8)	0.0273 (6)	0.0269 (6)	0.0175 (6)	0.0146 (6)	0.0119 (5)
C7	0.0360 (8)	0.0289 (7)	0.0260 (6)	0.0192 (6)	0.0153 (6)	0.0109 (5)
C8	0.0326 (8)	0.0347 (7)	0.0294 (7)	0.0152 (6)	0.0119 (6)	0.0102 (6)
C9	0.0364 (8)	0.0387 (8)	0.0287 (7)	0.0172 (7)	0.0075 (6)	0.0080 (6)
C10	0.0466 (9)	0.0422 (8)	0.0329 (7)	0.0217 (7)	0.0192 (7)	0.0192 (6)
C11	0.0342 (8)	0.0379 (8)	0.0320 (7)	0.0159 (7)	0.0142 (6)	0.0164 (6)
C12	0.0366 (8)	0.0331 (7)	0.0290 (7)	0.0210 (6)	0.0116 (6)	0.0083 (6)
C13	0.0298 (7)	0.0322 (7)	0.0300 (7)	0.0187 (6)	0.0150 (6)	0.0129 (5)
C14	0.0387 (8)	0.0330 (7)	0.0326 (7)	0.0155 (7)	0.0110 (6)	0.0139 (6)
C15	0.0445 (10)	0.0408 (9)	0.0335 (8)	0.0149 (8)	0.0079 (7)	0.0089 (7)
C16	0.0498 (10)	0.0602 (11)	0.0316 (8)	0.0290 (9)	0.0141 (7)	0.0216 (8)
C17	0.0557 (11)	0.0527 (10)	0.0442 (9)	0.0311 (9)	0.0271 (8)	0.0316 (8)
C18	0.0406 (9)	0.0327 (7)	0.0407 (8)	0.0191 (7)	0.0205 (7)	0.0166 (6)

*Geometric parameters (Å, °)*

Cl1—C3	1.7400 (15)	C8—C9	1.5167 (19)
O1—C7	1.4338 (17)	C8—H8A	0.9900
O1—H1O	0.823 (15)	C8—H8B	0.9900
O2—C12	1.2376 (19)	C9—H9A	0.9900
O3—C12	1.2560 (18)	C9—H9B	0.9900
N1—C10	1.485 (2)	C10—C11	1.514 (2)
N1—C9	1.487 (2)	C10—H10A	0.9900
N1—H1NB	0.861 (10)	C10—H10B	0.9900
N1—H1NA	0.873 (10)	C11—H11A	0.9900
C1—C2	1.383 (2)	C11—H11B	0.9900
C1—C6	1.393 (2)	C12—C13	1.5064 (19)
C1—H1A	0.9500	C13—C14	1.389 (2)
C2—C3	1.376 (2)	C13—C18	1.391 (2)
C2—H2A	0.9500	C14—C15	1.381 (2)
C3—C4	1.373 (3)	C14—H14A	0.9500
C4—C5	1.391 (2)	C15—C16	1.381 (2)
C4—H4A	0.9500	C15—H15A	0.9500
C5—C6	1.387 (2)	C16—C17	1.373 (3)
C5—H5A	0.9500	C16—H16A	0.9500
C6—C7	1.5250 (18)	C17—C18	1.386 (2)
C7—C8	1.533 (2)	C17—H17A	0.9500
C7—C11	1.536 (2)	C18—H18A	0.9500
C7—O1—H1O	114.0 (15)	N1—C9—H9A	109.4
C10—N1—C9	111.70 (12)	C8—C9—H9A	109.4
C10—N1—H1NB	110.7 (13)	N1—C9—H9B	109.4
C9—N1—H1NB	110.2 (13)	C8—C9—H9B	109.4
C10—N1—H1NA	108.5 (13)	H9A—C9—H9B	108.0
C9—N1—H1NA	110.3 (13)	N1—C10—C11	110.57 (13)
H1NB—N1—H1NA	105.3 (16)	N1—C10—H10A	109.5
C2—C1—C6	121.38 (14)	C11—C10—H10A	109.5
C2—C1—H1A	119.3	N1—C10—H10B	109.5

C6—C1—H1A	119.3	C11—C10—H10B	109.5
C3—C2—C1	118.85 (15)	H10A—C10—H10B	108.1
C3—C2—H2A	120.6	C10—C11—C7	112.01 (13)
C1—C2—H2A	120.6	C10—C11—H11A	109.2
C4—C3—C2	121.62 (14)	C7—C11—H11A	109.2
C4—C3—C11	119.92 (13)	C10—C11—H11B	109.2
C2—C3—C11	118.46 (13)	C7—C11—H11B	109.2
C3—C4—C5	118.82 (15)	H11A—C11—H11B	107.9
C3—C4—H4A	120.6	O2—C12—O3	124.52 (14)
C5—C4—H4A	120.6	O2—C12—C13	118.42 (13)
C6—C5—C4	121.26 (15)	O3—C12—C13	117.06 (13)
C6—C5—H5A	119.4	C14—C13—C18	118.72 (13)
C4—C5—H5A	119.4	C14—C13—C12	120.11 (13)
C5—C6—C1	118.06 (13)	C18—C13—C12	121.12 (13)
C5—C6—C7	122.92 (13)	C15—C14—C13	120.57 (14)
C1—C6—C7	119.01 (12)	C15—C14—H14A	119.7
O1—C7—C6	110.41 (11)	C13—C14—H14A	119.7
O1—C7—C8	108.40 (12)	C16—C15—C14	120.02 (16)
C6—C7—C8	112.93 (11)	C16—C15—H15A	120.0
O1—C7—C11	106.31 (12)	C14—C15—H15A	120.0
C6—C7—C11	110.12 (12)	C17—C16—C15	120.19 (15)
C8—C7—C11	108.43 (11)	C17—C16—H16A	119.9
C9—C8—C7	112.22 (12)	C15—C16—H16A	119.9
C9—C8—H8A	109.2	C16—C17—C18	119.94 (14)
C7—C8—H8A	109.2	C16—C17—H17A	120.0
C9—C8—H8B	109.2	C18—C17—H17A	120.0
C7—C8—H8B	109.2	C17—C18—C13	120.54 (15)
H8A—C8—H8B	107.9	C17—C18—H18A	119.7
N1—C9—C8	111.13 (12)	C13—C18—H18A	119.7
C6—C1—C2—C3	−0.1 (2)	C10—N1—C9—C8	−56.75 (16)
C1—C2—C3—C4	−0.1 (2)	C7—C8—C9—N1	55.69 (16)
C1—C2—C3—C11	−179.23 (12)	C9—N1—C10—C11	57.50 (16)
C2—C3—C4—C5	0.0 (3)	N1—C10—C11—C7	−57.35 (17)
C11—C3—C4—C5	179.15 (13)	O1—C7—C11—C10	−61.50 (15)
C3—C4—C5—C6	0.3 (3)	C6—C7—C11—C10	178.89 (12)
C4—C5—C6—C1	−0.5 (2)	C8—C7—C11—C10	54.87 (16)
C4—C5—C6—C7	−179.69 (14)	O2—C12—C13—C14	−173.36 (15)
C2—C1—C6—C5	0.4 (2)	O3—C12—C13—C14	6.1 (2)
C2—C1—C6—C7	179.65 (13)	O2—C12—C13—C18	3.9 (2)
C5—C6—C7—O1	114.43 (16)	O3—C12—C13—C18	−176.65 (15)
C1—C6—C7—O1	−64.80 (17)	C18—C13—C14—C15	−1.0 (2)
C5—C6—C7—C8	−7.11 (19)	C12—C13—C14—C15	176.34 (15)
C1—C6—C7—C8	173.66 (13)	C13—C14—C15—C16	0.7 (3)
C5—C6—C7—C11	−128.48 (15)	C14—C15—C16—C17	0.6 (3)
C1—C6—C7—C11	52.29 (16)	C15—C16—C17—C18	−1.5 (3)
O1—C7—C8—C9	61.09 (15)	C16—C17—C18—C13	1.1 (3)
C6—C7—C8—C9	−176.24 (11)	C14—C13—C18—C17	0.1 (2)

C11—C7—C8—C9	−53.92 (15)	C12—C13—C18—C17	−177.21 (14)
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*Hydrogen-bond geometry (Å, °)*

Cg3 is the centroid of the C13–C18 ring.

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
N1—H1 <i>NA</i> $\cdots$ O3 <sup>i</sup>	0.87 (1)	1.84 (1)	2.6964 (17)	166 (2)
O1—H1 <i>O</i> $\cdots$ O3	0.82 (2)	2.05 (2)	2.7780 (16)	147 (2)
N1—H1 <i>NB</i> $\cdots$ O2 <sup>ii</sup>	0.86 (1)	1.92 (1)	2.7609 (18)	166 (2)
C16—H16 <i>A</i> $\cdots$ C11 <sup>iii</sup>	0.95	2.78	3.5268 (17)	136
C9—H9 <i>B</i> $\cdots$ O1 <sup>i</sup>	0.99	2.46	3.3008 (19)	143
C1—H1 <i>A</i> $\cdots$ Cg3 <sup>iv</sup>	0.95	2.70	3.554 (2)	150

Symmetry codes: (i)  $-x+1, -y+1, -z+2$ ; (ii)  $x, y-1, z$ ; (iii)  $-x, -y+1, -z$ ; (iv)  $-x, -y+1, -z+1$ .